Performance Report

Title of Grant: Carbon Nanotubules: Building Blocks for Nanometer-Scale Engineering

Type of Report: Yearly Performance Report

Principle Investigator: Susan B. Sinnott

Period Covered: January 1, 1997 - November 1, 1997

Grantee's Institution: University of Kentucky
Department of Chemical and Materials Engineering
177 Anderson Hall
Lexington, Kentucky 40506-0046

Grant Number: NAG 2-1121

The proposed work consisted of two projects: the investigation of fluid permeation and diffusion through ultrafiltration membranes composed of carbon nanotubules and the design and study of molecular transistors composed of nanotubules. Below I will outline the progress being made on each project and also discuss an additional project that is a continuation of work supported by an 1995-1996 NASA Ames Computer grant.

1) Liquid Interactions within a Nanotubule Membrane:

A) The first goal was to characterize the interactions of polar liquid molecules that might be important in pharmaceutical ultrafiltration processes with carbon nanotubules. This is being done with electronic structure calculations using density functional theory within the pseudopotential approximation. In addition, we are investigating the charge transfer that occurs between various molecules and tubule walls. This is important for two reasons: it is representative of salts that might be present in pharmaceutical systems and it is related to experimental work taking place at the University of Kentucky to disperse nanotubule fibers in polymer matrices.

B) The second goal was to modify the many-body, empirical hydrocarbon potential developed by Brenner to include oxygen atoms. This work is progressing extremely well and we plan on testing our preliminary potential within the next month. The inclusion of charge transfer between oxygen, carbon and hydrogen will take slightly longer however, as this step requires modification of the original hydrocarbon potential. We anticipate starting the large-scale molecular dynamics simulations using this potential after it has been fully tested and before the charge transfer has been completely included. This will allow us to eventually determine the effect of

charge transfer on the simulation results. When the potential is finished and we have confidence that it has been fully tested and is reliable, it will be made available to anyone who wants to use it.

2) Design of Nanometer-Scale Hydrocarbon Electronic Devices

We have performed a series of tight-binding calculations on the electronic properties of straight nanotubule junctions. We have also had several conversations with Robert Haddon, who last April left Lucent Technologies to accept a position as a Professor of Chemistry at the University of Kentucky. He has been working on the dispersion of nanotubules in polymer matrices (mentioned above). He is also working on making electronic devices using organic systems in place of silicon and he remains interested in our work.

3) Mechanical Properties of Nanotubules and Nanotubule Bundles

In 1995 we obtained a NAS computer time grant to study the mechanical properties of nanotubule bundles. We found that when the bundle is composed of small-diameter tubules packed closely together, it can be more stiff in the direction of the tubule axis than diamond. This led to the design of a nanotubule-diamond composite that takes advantage of the nanotubule bundle's high modulus and stabilizes the bundle against shear stresses. We used our computer time to perform molecular dynamics simulations of the shear and tensile deformation of the composite and determined that it is quite stable to these forces.[1]

This work led us to reexamine the question of the mechanical properties of single nanotubules. We therefore are investigating the deformation mechanisms and Euler buckling forces of nanotubules that are used as proximal probe tips and are indented on diamond and graphite surfaces. This is a process that Smalley and co-workers recently demonstrated was feasible experimentally.[2] We find that Euler buckling forces for shorter nanotubules are much higher than for longer nanotubules even though the modulus is the same in each case.[3]

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[1] S. B. Sinnott, O. A. Shenderova, C. T. White, D. W. Brenner, *Carbon* (in press).

[2] H. Dai, J. H. Hafner, A. G. Rinzler, D. T. Colbert and R. E. Smalley, Nature **384,** 147 (1996).

[3] A. Garg and S. B. Sinnott, *Nanotechnology* (submitted 10/15/97).

Publications to Date:

"Engineering of Nanostructures from Carbon Nanotubules", A. Garg and S. B. Sinnott, *Nanotechnology* (submitted 10/15/97).

Abstract

Proximal probe technology has provided researchers with new ways to investigate and manipulate matter on the nanometer scale. We have studied, through molecular dynamics simulations, using a many-body empirical potential, the indentation of a hydrogen-terminated, diamond (111) surface, with a proximal probe tip that consists of an open, hydrogen-terminated, (10,10) carbon nanotubule. The simulations showed that upon indenting 1.8 Å, the tubule deforms but returns to its original shape upon retraction. The Young's modulus of the tubule was determined using the predicted Euler buckling force and was found to be comparable to measured and calculated values. In a second series of simulations, an open (10, 10) nanotubule was heated to 4500 K and allowed to close. We find that at this temperature the resulting cap contains numerous imperfections, including some not mentioned previously in the literature.

Other Media in which the Research was Discussed:

1) Invited Seminar titled "Atomistic Simulations to Investigate the Nanometer-Scale Properties of Materials", S. B. Sinnott, The Department of Physics, Virginia Commonwealth University in Richmond, VA, April 4, 1997.

2) Invited Technical presentation titled "Engineering of Nanostructures from Carbon Nanotubules", S. B. Sinnott, Sixth Annual Consortium on Nanostructured Materials, Lexington, Kentucky, October 24, 1997.

3) Publication of the Abstract for the Fifth Foresight Conference on Molecular Technology in addition to the draft of the Nanotechnology paper mentioned above on the World Wide Web titled "Engineering of Nanostructures from Carbon Nanotubules", S. B. Sinnott and A Garg.
   See: http://www.foresight.org/Conferences/MNT05/Abstracts/Sinnabst.html
   and http://www.foresight.org/Conferences/MNT05/Papers/Sinnott/index.html